

and nano scales before grafting biomolecules. To do that, we used complementary methods such as X-ray Photoelectron Spectroscopy (XPS), Polarization Modulation-Infrared Reflection Adsorption Spectroscopy (PM-IRRAS), contact angle and Atomic Force Microscopy (AFM). Among all these techniques, only the AFM allows us to analyze the samples at the nanoscale. Herein we present a set of results on the characterization and comparison of various SAMs on gold. In particular, the AFM investigation has allowed us to get into the homogeneity and the adhesion properties of the samples.

[1]. M. Veiseh, B.T. Wickes, D.G. Castner, M. Zhang *Biomaterials* 25 (2004) 3315-3324.

[2]. J. Lahiri, L. Isaacs, J. Tien, G.M. Whitesides, *Anal. Chem.* 71 (1999) 777790.

[3]. The ANR P2N (ANR-12-NANO-0016-04 - PIRANEX project) is greatly acknowledged for financial support; CNANO Rhône-Alpes for PM-IRRAS funding; NanoLyon for providing gold samples

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Sublattice localized electronic states in atomically resolved graphene-Pt(111) edge-boundaries

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Understanding the connection of graphene with metal surfaces [1] is a necessary step for developing atomically-precise graphene-based technology. In this work [2] we combine high resolution RT-STM experiments with DFT calculations and non-equilibrium Green's functions method to unveil the atomic structure of a border-like edge between a Pt(111) step and a graphene zigzag edge. We have managed to get atomic resolution not only on both the metal and the graphene but also on the boundary (see Fig. 1). The graphene edges minimize their strain by inducing a 3-fold edge-reconstruction on the metal side. The tendency to form passivated zigzag graphene terminations plays a relevant role in the formation and orientation of the stable Moiré patterns. Our combined approach reveals the interesting electronic properties of this nanoscopic system including the preservation of the G-edge state shifted to energies at about +0.8 eV above Fermi level, highly localized in one of the graphene sublattices and confined to the G-Pt interface. This state spreads out inside the first Pt row resulting in a high quality G-metal electric contact that could be relevant for designing future atomically precise graphene metal leads [3].

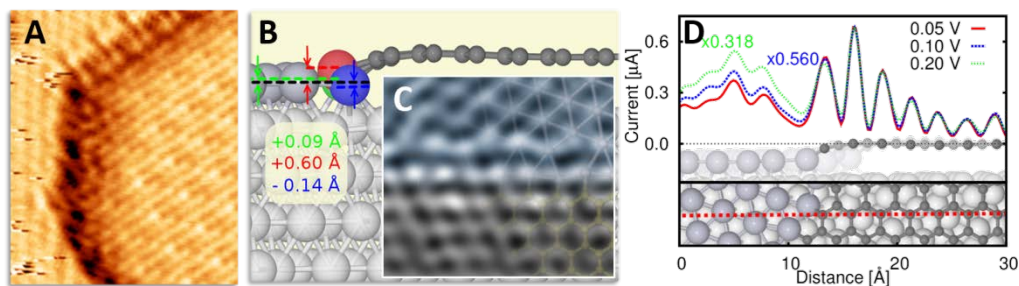


Fig. 1 A) Experimental RT-STM image of a graphene flake on a Pt(111) step edge. B) Atomic structure of graphene zigzag edge on a Pt step calculated by a DFT method based on VASP. C) STM image compared with the atomic structure calculated with DFT. D) Simulated STM profiles at constant height (2.75 Å) for different bias voltages.

[1]. P. Sutter et al, PRB, **80**, 245411 (2009); Martínez-Galera et al., Nano Lett., **11**, 3576 (2011).

[2]. P. Merino, L. Rodrigo et al. Accepted in ACS Nano (DOI: 10.1021/nn500105a).

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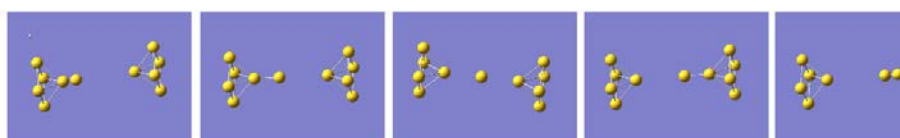
Quantum Capacitance and Electromigration: A Theoretical Approach

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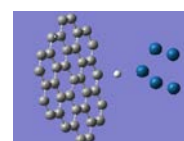
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In recent years electron transport through metallic contacts at the nanoscale has been studied theoretically and with experiments. The most studied quantity is the current along with its derivatives. However, this is not the only quantity that can be measured. Capacitance also gives valuable information about the electronic and structural properties of the nanocontacts. We are interested here in the Quantum Capacitance which depends on the density of states and measures the quantum contribution to the capability of a device to accumulate electrons. This quantity depends of the chemical nature, i.e., of the available atomic levels of the material. It also depends of the energy with which electrons are injected. Therefore, it has a quantum mechanical origin in contrast to the purely electrostatic one^[1].

We used ab-initio calculations based on DFT methods and the Nonequilibrium Green's Function Formalism to simulate such systems. To introduce non-equilibrium conditions, we apply an external bias voltage, at which electrons are injected. Among the simulated systems, there are contacts from different metals. Non-voltage-symmetric charge distributions emerge of our calculations. This is a result of the absence of electron-hole symmetry. The distinctive DOS corresponding to each metal is determinant in the capacitance, as well as other transport properties.



Simulation of Gold atom electromigration between two contacts under applied bias voltage.



Chemisorption of H on Graphene.